Ethyl hydrogen glutarate

1070-62-8 | DTXSID20147865

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 279 °C

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 5.22e-01

Nearest Neighbors from the Training Set

Image not found

Hexanoic acid, 5-oxo-
Measured: 275
Predicted: 247

Image not found

9-Cycloheptadecen-1-one
Measured: 343
Predicted: 330

Image not found

Cyclohexaneacetic acid
Measured: 245
Predicted: 245

Image not found

1-Cyclohexenecarboxylic acid
Measured: 241
Predicted: 241